

# Short-range defects contribution to the monolayer graphene resistivity

Natalie E. Firsova

*Institute for Problems of Mechanical Engineering,  
the Russian Academy of Sciences, St. Petersburg 199178, Russia*

Sergey A. Ktitorov

*A.F. Ioffe Physical-Technical Institute, the Russian Academy of Sciences, St. Petersburg, Russia*

The derived by us earlier electron scattering matrix for the short-range defects in monolayer graphene is applied to description of the resistivity electron density dependence. It is argued that large charged defect density is unlikely in the suspended graphene and graphene lying above the trench.

## I. INTRODUCTION

Electronic states in monolayer graphene with point defects were considered in [1], [2], [3] and in our works [4], [5]. The main novel element in our works is the band asymmetry of the defect potential in the Dirac equation. This asymmetry appears naturally if the defect violates the symmetry between the sublattices. This asymmetry was described in terms of equivalent superposition the band-symmetric potential and the mass (gap) perturbations. Characteristic equations for the energy eigenvalues for the gapped graphene and complex energies for resonances were derived and analysed. Exact formulae for the scattering and transfer matrices were obtained. Important features of the electronic states in the presence of the asymmetric potential were found in [6]. Our goal in this work is to study the impact of these features on the electronic transport in the monolayer graphene.

## II. BASIC EQUATIONS

The Dirac equation describing electronic states in zero-gap graphene reads [6]

$$\left( -iv_F \hbar \sum_{\mu=1}^2 \sigma_{\mu} \partial_{\mu} - \sigma_3 \delta m v_F^2 \right) \psi = (E - V) \psi, \quad (1)$$

where  $v_F$  is the Fermi velocity,  $\sigma_{\mu}$  are the Pauli matrices,  $\psi(\mathbf{r})$  is the two-component spinor. The spinor structure takes into account the two-sublattice structure of graphene.  $\delta m(\mathbf{r})$  and  $V(\mathbf{r})$  are the local perturbations of the mass (gap) and the chemical potential. A local mass perturbation can be induced by defects in the graphene film or in the substrate. The perturbation matrix elements

$$\text{diag}(V_1, V_2) r_0 \delta(r - r_0) \quad (2)$$

are related to the  $a, b$  parameters as follows

$$-V_1 = a + b, \quad -V_2 = a - b \quad (3)$$

The delta function perturbation is the simplest solvable short-range model. Finite radius  $r_0$  plays a role of the regulator and is necessary in order to exclude deep states of the atomic energy scale. The finite perturbation radius  $r_0$  leads to the quasi-momentum space form-factor proportional to the Bessel function that justifies our neglect of transitions between the Brillouin band points  $K$  and  $K'$ .

Let us introduce dimensionless variables and parameters:

$$\epsilon = \frac{E}{\hbar v_F / r_0}, \quad \tilde{m} = \frac{m v_F^2}{\hbar v_F / r_0}, \quad u_i = \frac{V_i}{\hbar v_F / r_0}, \quad i = 1, 2, \quad \tilde{\mathbf{r}} = \frac{\mathbf{r}}{r_0}, \quad \tilde{\partial}_{\mu} = \frac{\partial}{\partial \tilde{\mathbf{r}}}, \quad (4)$$

$$r_0 \delta(r - r_0) = \delta(\tilde{r} - 1). \quad (5)$$

The equation (1) takes the form

$$\left( -i \sum_{\mu=1}^2 \sigma_{\mu} \tilde{\partial}_{\mu} + \sigma_3 \tilde{m} - \sigma_3 \delta \tilde{m} \right) \psi = (\epsilon - u) \psi, \quad (6)$$

We confine ourselves here by the case of zero-gap graphene;  $\tilde{m} = 0$ .  
Let us present the two-component spinor in the form

$$\psi_j(\tilde{\mathbf{r}}, t) = \frac{\exp(-iEt)}{\sqrt{\tilde{r}}} \begin{pmatrix} f_j(\tilde{r}) \exp[i(j-1/2)\phi] \\ g_j(\tilde{r}) \exp[i(j+1/2)\phi] \end{pmatrix}, \quad (7)$$

where  $j$  is the pseudospin quantum number;  $j = \pm 1/2, \pm 3/2, \dots$ . In the opposite to the relativistic theory, this quantum number has nothing to do with the real spin and indicates the degeneracy in the biconic Dirac point. The upper  $f_j(r)$  and lower  $g_j(r)$  components of the spinor satisfy the equations

$$\frac{dg_j}{d\tilde{r}} + \frac{j}{\tilde{r}}g_j + \epsilon f_j = (a+b)\delta(\tilde{r}-1)f_j, \quad (8)$$

$$-\frac{df_j}{d\tilde{r}} + \frac{j}{\tilde{r}}f_j - \epsilon g_j = (a-b)\delta(\tilde{r}-1)g_j. \quad (9)$$

The general solution can be found solving the second-order equation obtained by excluding one of the spinor components from the equation set (8), (9) in the domains  $0 < r < r_0$  and  $r > r_0$ :

$$\frac{d^2 f_j}{d\tilde{r}^2} + \left[ \epsilon^2 - \frac{j(j-1)}{\tilde{r}^2} \right] f_j = 0. \quad (10)$$

This equation is related to the Bessel one. Its general solution in the domain  $0 < r < r_0$  reads

$$f_j = C_1 \sqrt{\epsilon \tilde{r}} J_{j-1/2}(\epsilon \tilde{r}) + C_2 \sqrt{\epsilon \tilde{r}} N_{j-1/2}(\epsilon \tilde{r}), \quad (11)$$

where  $J_\nu(z)$  and  $N_\nu(z)$  are the Bessel and Neumann functions respectively. The constant  $C_2$  vanishes in the domain  $0 \leq \tilde{r} < 1$  since the solution must be regular at the origin. The solution in the region  $\tilde{r} \geq 1$  reads

$$f_j = C_3 H_{j-1/2}^{(1)}(\epsilon \tilde{r}) + C_4 H_{j-1/2}^{(1)}(\epsilon \tilde{r}),$$

where  $H_\nu^{(\alpha)}(z)$  is Hankel's function. Matching these solutions at the circumference of the circle of radius  $r = r_0$  ( $\tilde{r} = 1$ ) we obtain a scattering matrix and a characteristic equation for the resonance states. Calculating the ratio of the out-going and in-going waves, we obtain the S-matrix components in the angular momentum representation (for details see [5]):

$$S_j(\epsilon) = -\frac{\mathcal{F}_j^{(2)}}{\mathcal{F}_j^{(1)}}, \quad (12)$$

where  $\mathcal{F}_j^{(\alpha)}$  is given by the formula:

$$\begin{aligned} \mathcal{F}_j^{(\alpha)} = & \left( J_{j-1/2}(\epsilon) H_{j+1/2}^{(\alpha)}(\epsilon) - J_{j+1/2}(\epsilon) H_{j-1/2}^{(\alpha)}(\epsilon) \right) - \\ & \left[ (a-b) J_{j+1/2}(\epsilon) H_{j+1/2}^{(\alpha)}(\epsilon) + (a+b) J_{j-1/2}(\epsilon) H_{j-1/2}^{(\alpha)}(\epsilon) \right], \\ & \alpha = 1, 2. \end{aligned} \quad (13)$$

Poles of the scattering matrix (12) are determined by the characteristic equation

$$\mathcal{F}_j^{(1)}(\epsilon) = 0, \quad (14)$$

or

$$(a-b) J_{j+1/2}^2(\epsilon) + (a+b) J_{j-1/2}^2(\epsilon) = i \left[ (a-b) J_{j+1/2}(\epsilon) N_{j+1/2}(\epsilon) + (a+b) J_{j-1/2}(\epsilon) N_{j-1/2}(\epsilon) \right] = -i \frac{2}{\pi \epsilon} \quad (15)$$

### III. ANALYSIS OF THE CHARACTERISTIC EQUATION AND CALCULATION OF THE CONDUCTIVITY

Using the relations  $H_n^{(1)}(z) = J_n + iN_n$ ,  $H_n^{(2)} = J_n - iN_n$ , we can write S-matrix in the form:

$$S_j(\epsilon) = -\frac{A_j(\epsilon) - iB_j(\epsilon)}{A_j(\epsilon) + iB_j(\epsilon)} = \frac{B_j(\epsilon) + iA_j(\epsilon)}{B_j(\epsilon) - iA_j(\epsilon)}, \quad (16)$$

and, therefore, it can be presented in the standard form [?] ]

$$S_j(\epsilon) = \exp[i2\delta_j(\epsilon)], \quad (17)$$

where the scattering phase is given by the expression

$$\delta_j(\epsilon) = \arctan \frac{A_j(\epsilon)}{B_j(\epsilon)}. \quad (18)$$

Formulae (16), (17) show that the scattering matrix  $S_j(\epsilon)$  is unitary on the continuum spectrum. The functions  $A_j(\epsilon)$  and  $B_j(\epsilon)$  are determined as follows

$$A_j(\epsilon) = -\left[(a+b)J_{j-1/2}^2(\epsilon) + (a-b)J_{j+1/2}^2(\epsilon)\right], \quad (19)$$

$$B_j(\epsilon) = -\frac{2}{\pi\epsilon} \left[(a+b)J_{j-1/2}(\epsilon)N_{j-1/2}(\epsilon) + (a-b)J_{j+1/2}(\epsilon)N_{j+1/2}(\epsilon)\right] + \\ [J_{j+1/2}(\epsilon)N_{j-1/2}(\epsilon) - J_{j-1/2}(\epsilon)N_{j+1/2}(\epsilon)] \quad (20)$$

Asymptotic behaviour of the scattering phases and other scattering data at  $\epsilon \rightarrow 0$  can be obtained expanding the cylinder functions for small arguments [7]:

$$J_n(z) \sim \frac{1}{n!} (z/2)^2, \quad N_n(z) = \begin{cases} -\frac{\Gamma(n)}{\pi} (2/z)^n & \text{for } n > 0, \\ (2/\pi) \log(\gamma_E z/2) & \text{for } n = 0, \end{cases} \quad z \rightarrow 0, \quad (21)$$

where  $\gamma_E \approx 0,577$  is the Eyler-Masceroni constant,  $\Gamma(n)$  is the gamma-function. Then we have for the scattering phases in the lower order in  $\epsilon$ :

$$\tan \delta_{\pm 1/2} \approx (b \pm a) \frac{\pi}{2}\epsilon, \quad \epsilon \rightarrow 0, \quad (22)$$

$$\tan \delta_{\pm(n+1/2)} \approx \pm\pi (\epsilon/2)^{2n+1} (b \pm a) \quad \epsilon \rightarrow 0. \quad (23)$$

The transport cross section can be written in terms of the scattering phases [3] (we have returned to dimensional variables here)

$$\Xi_{tr} = \frac{2r_0}{\epsilon} \sum_{j=\pm\frac{1}{2}, \pm\frac{3}{2}, \dots} \sin^2(\delta_{j+1} - \delta_j). \quad (24)$$

The transport relaxation time can be calculated using the following relation:

$$1/\tau_{tr} = N_I v_F \Xi_{tr}. \quad (25)$$

Taking into account the approximate formulae for phases (22), (23), the series (24) can be written in the following asymptotic form for  $\epsilon \rightarrow 0$ :

$$\Xi_{tr} = \frac{2r_0}{\epsilon} \left[ (\delta_{1/2} - \delta_{-1/2})^2 + (\delta_{3/2} - \delta_{1/2})^2 + (\delta_{-3/2} - \delta_{-1/2})^2 + \dots \right. \\ \left. (\delta_{n+1/2} - \delta_{n-1/2})^2 + (\delta_{-n-1/2} - \delta_{-n+1/2})^2 + \dots \right] \approx \epsilon r_0 \pi^2 [2a^2 + O(\epsilon)]. \quad (26)$$

Then the asymptotic formula for the transport relaxation time reads:

$$1/\tau_{tr} = \epsilon N_I v_F \pi^2 2a^2 [1 + O(\epsilon)] \quad (27)$$

It is seen from (27) that asymptotic behaviour of the relaxation time at  $\epsilon \rightarrow 0$  is determined by the parameter  $a$ , i. e. by the symmetric component of the perturbation.

Let us consider now the Born approximation for the scattering amplitude. The partial wave series for the transport cross section converges rather slowly. That is why we consider a behaviour of the transport cross section without the partial wave expansion. In return we can use the Born approximation in this limit. The Born formula for the scattering amplitude reads [3]:

$$f^{Born}(p, \theta) = -\frac{1}{\hbar v_F} \sqrt{\frac{p}{8\pi}} V(\mathbf{q}), \quad (28)$$

where  $\hbar \mathbf{q} = \hbar \mathbf{p} - \hbar \mathbf{p}'$  is the transferred momentum,  $q = 2p \sin \theta/2$ ,  $V(\mathbf{q})$  is the perturbation Fourier transform:

$$V(\mathbf{q}) = \int d^2r e^{-i\mathbf{q}\mathbf{r}} V(\mathbf{r}) = \int_0^\infty dr r V(r) \int_0^{2\pi} d\phi \exp[-iqr \cos \phi] = 2\pi \int_0^\infty dr r V(r) J_0(qr). \quad (29)$$

Inserting the potential (2) into (29) we obtain

$$V_i(\mathbf{q}) \equiv V(p, \theta) = 2\pi V_i^0 r_0^2 J_0(2pr_0 \sin \theta/2). \quad (30)$$

Substituting (30) into (28) we obtain the scattering amplitude:

$$f_i^{Born}(p, \theta) = -\frac{2\pi r_0^2 V_i^0}{\hbar v_F} \sqrt{\frac{p}{8\pi}} J_0(2pr_0 \sin \theta/2), \quad (31)$$

Now we can calculate the transport cross section [3]:

$$\Xi_{tr}^{Born} = \int_0^\pi d\theta (1 - \cos \theta) |f^{Born}(p, \theta)|^2 = (pr_0) r_0 \left( \frac{V_i^0}{\hbar v_F / r_0} \right)^2 \pi/2 \int_0^\pi d\theta (1 - \cos \theta) J_0^2(2pr_0 \sin \theta/2). \quad (32)$$

This integral can be expressed in terms of the hypergeometric functions [7]:

$$\int_0^\pi d\theta (1 - \cos \theta) J_0^2(2pr_0 \sin \theta/2) = \Gamma \left( \begin{matrix} 1/2, & 3/2 \\ 2, & 1, & 1 \end{matrix} \right) \cdot {}_3F_4 \left( 3/2, 1/2, 1, 2, 1, 1, 1; - (2pr_0)^2 \right), \quad (33)$$

where  $\Gamma \left( \begin{matrix} \alpha_1, & \alpha_2 \\ \beta_1, & \beta_2, & \beta_3 \end{matrix} \right) \equiv \frac{\Gamma(\alpha_1)\Gamma(\alpha_2)}{\Gamma(\beta_1)\Gamma(\beta_2)\Gamma(\beta_3)}$ ,  $\Gamma(\alpha)$  is the gamma function,  ${}_3F_4(\alpha_1, \alpha_2, \alpha_3; \beta_1, \beta_2, \beta_3, \beta_4; x)$  is the generalized hypergeometric function. It is determined by the series [7]:

$${}_3F_4(\alpha_1, \alpha_2, \alpha_3; \beta_1, \beta_2, \beta_3, \beta_4; x) = \sum_{k=0}^{\infty} \frac{(\alpha_1)_k (\alpha_2)_k (\alpha_3)_k}{(\beta_1)_k (\beta_2)_k (\beta_3)_k (\beta_4)_k} \frac{x^k}{k!}, \quad (34)$$

where  $(\alpha)_k = \frac{\Gamma(\alpha+k)}{\Gamma(\alpha)}$  is the rising Pochhammer symbol. When  $pr_0 < 1$ , we can neglect all higher terms of this series and obtain in result the transport scattering cross section  $\Xi_{tr}^{Born} \sim pr_0$ . Notice that the Born approximation is here asymptotically exact in the limit  $pr_0 \rightarrow 0$ . It must be noted here that the limit of  $pr_0$ ,  $E_F$ ,  $k_B T$ ,  $\hbar \omega$  tending to zero is obviously nontrivial and many-particle effects must be taken into account in this case. This problem will be not discussed here. The opposite limit of  $pr_0 > 1$  is not actual for scattering on rare point defects. It can be urgent for the model of random potential with large correlation radius and for the quantum dot model, but they are outside of the scope of this work. However, there exist at least two other possibilities to obtain the cross section behaviour, different from the power law  $\Xi_{tr}^{Born} \sim pr_0$ . First of them corresponds to a random potential with the correlation radius  $r_0 \gg a$ . In this case one can consider scattering of electrons with  $pr_0 \sim 1$ . Another possibility is related to the resonance scattering studied in our works [5]. We analyse here the latter case.

Let us consider the limit of large angular momentum  $j \gg 1$  using the Bessel function asymptotics:

$$J_\nu(z) \sim \frac{1}{\sqrt{2\pi\nu}} \left(\frac{ez}{2\nu}\right)^\nu (1 + O(1/\nu)), \quad \nu \rightarrow \infty, \quad (35)$$

$$N_\nu(z) \sim -\sqrt{\frac{2}{\pi\nu}} \left(\frac{ez}{2\nu}\right)^{-\nu} (1 + O(1/\nu)), \quad \nu \rightarrow \infty, \quad (36)$$

$$H_\nu^{(1)}(z) \sim \frac{1}{\sqrt{2\pi\nu}} \left[ \left(\frac{ez}{2\nu}\right)^\nu - 2i \left(\frac{ez}{2\nu}\right)^{-\nu} \right] (1 + O(1/\nu)), \quad \nu \rightarrow \infty, \quad (37)$$

where  $e$  is the base of natural logarithms. The characteristic equation 15 takes the following form in the limit of  $j \gg 1$ :

$$\frac{a-b}{(2j+1)(2j-1)^{2j+2}} (e\epsilon)^{2j+2} + \frac{a+b}{(2j-1)(2j-1)^{2j}} (e\epsilon)^{2j} = ie \left[ \frac{\epsilon}{2j-1} \left( \frac{a-b}{j+1/2} + \frac{a+b}{j-1/2} \right) - \frac{2}{2j-1} \right], \quad (38)$$

Applying the same approach to the scattering

Our numerical analysis shows that the energy dependence of the relaxation time crosses over to an approximate constant at high energy, and position of the crossing-over point depends on the ratio  $a/b$  (see fig. 1). The Boltzmannian conductivity is determined by the formula:

$$\sigma = \frac{e^2}{h} (E_F \tau_{tr} / \hbar), \quad (39)$$

where  $\tau_{tr}$  is determined as follows

$$\tau_{tr}^{-1} = N_I \Sigma_{tr} v_F. \quad (40)$$

The mobility can be determined as the ratio:

$$\mu = \frac{\sigma}{en}, \quad (41)$$

where the carrier density at low temperature is determined as follows

$$n = N/S = \frac{1}{2\pi} \left( \frac{E_F}{\hbar v_F} \right)^2 \quad (42)$$

Using (27), (39), and (40) we conclude that the conductivity tends to a constant value in the limit  $E_F \rightarrow 0$ . This limit must be considered taking into account the fact that the accepted here Boltzmann kinetics is invalid in the vicinity of the point  $E_F = 0$ . In the opposite limit of large  $E_F$ , we conclude using (??) and (40) instead of (27) that conductivity increases linearly with the Fermi energy in this energy region. The mobility behaves at small and large Fermi energy respectively as  $E_F^{-2}$  and  $E_F^{-1}$ .

- 
- [1] D.M. Basko, Phys. Rev. B 78 115432 (2008)
  - [2] Yu.G. Pogorelov, arXiv:cond-mat/0603327v1.
  - [3] D.S. Novikov, Phys. Rev. B 76 245435 (2007).
  - [4] Natalie E. Firsova, Sergey A. Kitorov, Philip A. Pogorelov, Physics Letters A **373**, 525 (2009)
  - [5] Natalie E. Firsova, Sergey A. Kitorov, Physics Letters A **374**, 1270 (2010).
  - [6] A.H. Castro Neto, F. Guinea, et al, arXiv: 0709.1163 (2008).
  - [7] M. Abramowitz, I.A. Stegun, *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables*, National Bureau of Standards, Washington DC, 1964.